LES SOFTWARE FOR THE DESIGN OF LOW EMISSION COMBUSTION SYSTEMS FOR VISION 21 PLANTS

Quarterly Technical Progress Report for

October – December 2004

by

Clifford E. Smith

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P.O. Box 10940
Pittsburgh, PA 15236

Technical Monitor: Mr. Norman T. Holcombe
Contract Monitor: Ms. Crystal Sharp

CFD Research Corporation www.cfdrc.com
215 Wynn Drive • Huntsville, Alabama 35805 • Tel: (256) 726-4800 • FAX: (256) 726-4806 • info@cfdrc.com

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ABSTRACT

The draft final report was written and delivered to DOE in January 2005. All work in the project was completed.

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1. INTRODUCTION

Vision 21 combustion systems will require innovative low emission designs and low development costs if Vision 21 goals are to be realized. In this three-year project, an advanced computational software tool will be developed for the design of low emission combustion systems required for Vision 21 clean energy plants. The combustion Large Eddy Simulation (LES) software will be able to accurately simulate the highly transient nature of gaseous-fueled turbulent combustion so that innovative concepts can be assessed and developed with fewer high-cost experimental tests. During the first year, the project included the development and implementation of improved chemistry (reduced GRI mechanism), subgrid turbulence (localized dynamic), and subgrid combustion-turbulence interaction (Linear Eddy) models into the CFD-ACE+ code. University expertise (Georgia Tech and UC Berkeley) was utilized to help develop and implement these advanced submodels into the unstructured, parallel CFD flow solver, CFD-ACE+. Efficient numerical algorithms that rely on *in situ* look-up tables or artificial neural networks were implemented for chemistry calculations. In the second year, the combustion LES software was evaluated and validated using experimental data from lab-scale and industrial test configurations. This code testing (i.e., alpha testing) was performed by CFD Research Corporation's engineers. During the third year, six industrial and academic partners used the combustion LES code and exercised it on problems of their choice (i.e., beta testing). Final feedback and optimizations were then be implemented in the final release version of the combustion LES software that will be licensed to the general public.

An additional one-year task was added for the fourth year of this program entitled, "LES Simulations of SIMVAL Results." For this task, CFDRC performed LES calculations of selected SIMVAL cases, and compared predictions with measurements. In addition to comparisons with NO_x and CO exit measurements, comparisons were made to measured pressure oscillations. Possible gaps in the data sets were identified, as well as potential areas of improvement for combustion and turbulence models.

2. EXECUTIVE SUMMARY

Work in this seventeenth quarter (October – December 2004) consisted of writing the draft final report for review by DOE. The report was delivered to DOE in January, 2005.

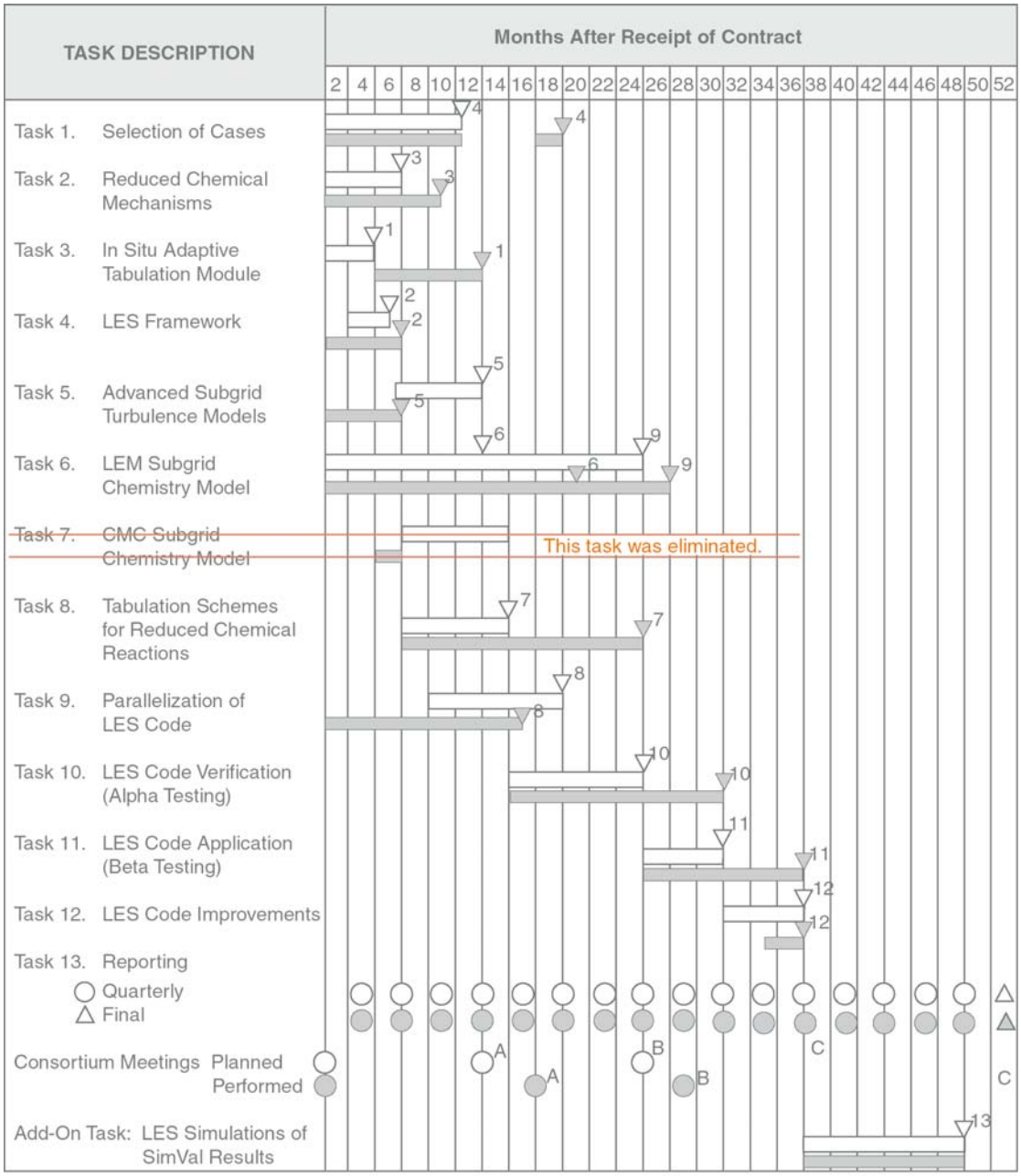
3. EXPERIMENTAL

No experiments were performed this quarter.

4. RESULTS

A draft final report was written and delivered to DOE in January, 2005.

APPENDIX A — WORK SCHEDULE



Key Milestones

1 Complete In-Situ Adaptive Tabulation Module
2 Complete LES Framework Modification to CFD-ACE+
3 Complete Reduced Mechanisms
4 Complete Selection of Cases
5 Complete Implementation of Turbulence Models
6 Complete Implementation of Initial Version of LEM Model
7 Complete Tabulation Schemes
8 Complete Parallelization of LES Code
9 Complete Implementation of LEM Model
10 Complete Alpha Testing of LES Code
11 Complete Beta Testing of LES Code
12 Final Release of LES Code
13 Complete SimVal Comparisons

Performance Targets

A Alpha Release of LES Code
B Beta Release of LES Code
C Final Commercial Release of LES Code

Planned
Performed

APPENDIX B — FUTURE PLANS

All work has been completed.